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Atomic Compton profile

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Abstract Atomic K and L-shell Compton-profiles for MoK_{α} radiation are studied within the framework of a form factor approximation by using screened hydrogenic wave functions. Numerical results presented for the lack of symmetry in the profile values about $q = 0$ (q is the usual Compton parameter) for atoms from $_{3}$Heto $_{18}$Ar are used to judge the quality of approximation methods for correcting the impulse double differential cross section for Compton scattering.

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When a radiation is Compton scattered, the emerging beam is Doppler broadened because of the motion of the target electron. The analysis of the broadened lineshape or the so-called Compton-profile provides detailed information about the electron momentum distribution in the target. The line profile $J(P_z)$ is determined by the probability that the scattering electron has a component momentum p_z, that is

$$J(p_z) = \int_{p_x} \int_{p_y} \chi^*(\boldsymbol{p})\, \chi(\boldsymbol{p})\, dp_x dp_y , \tag{1}$$

where $\chi(\boldsymbol{p})$ is the electron wave function in the momentum representation obtained by Fourier transformation of the real space wave function $\psi(\boldsymbol{r})$. Eq. (1) gives the expression in the impulse approximation which implies that the interaction between the photon and electron takes place in such a short time that the scattering interaction is over before the electron had had a chance to move in the potential well and change its potential energy. Naturally, the outgoing electron is represented here by a plane wave. The initial state of the electron is supposed to have a momentum $\boldsymbol{p}_i$ and energy $\frac{p_i^2}{2m}$, not the electron binding energy $-E_B$. The energy momentum conservation relation is expressed accordingly. However for a typical element, the above picture tends to break down at intermediate and small momentum transfers. One then takes course to an exact hydrogenic (EH) calculation [1], which consists in using more realistic final state wave functions than plane waves and introducing the electron binding energy to express the energy momentum conservation.

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The appropriate theory in respect of this was developed as early as 1934 by Felix Bloch [2]. But the topic did not receive much attention for quite a long time although there is no single identifiable reason to account for the sudden inactivity. In recent years there has been resurgence of interest in the exact Compton -profile calculation, which on the one hand, can give improved results over the corresponding impulse-model values and, on the other hand, can be used to examine the domain of validity of the impulse-model [3]. In an exact calculation [4] the Compton peak may move to slightly higher or lower energies when compared with the impulse profile and the lineshape may change. The inconsistency of the experimentally observed profile maximum with the prediction of the IA gave further stimulus for theoretical works. In the present paper, we shall try to clarify some of the conceptual aspects of the profile asymmetries.

In extending the theory of Wentzel [5], Bloch [2] first studied the scattering of photons from any initial hydrogenic bound state with the wave functions expressed in parabolic coordinate system. The exact hydrogenic results were, however, left in terms of residue integrals and their derivatives. These were not evaluated because of their complexities. After forty years, Bloch and Mendelsohn [6] re-examined and re-derived the theory of exact hydrogenic Compton profile in response to the needs of the contemporary experimental observations. They pointed out certain mathematical errors in the seminal work of Bloch [2] and also worked out the results for the residue integrals leading to closed form expression for the *EH* Compton profile.

The exact Compton-profile $J_{nl}^{EH}(q)$ for scattering of photon by an orbital electron (nl) of a hydrogenic system is given by

$$J_{nl}^{EH}(q) = \left|\frac{w_1}{w_2}\right| 27.212 k Z I_{nl}^{EH}(q)/n \tag{2}$$

The quantity k is related to the photon scattering vector and can be written as

$$k^2 = \frac{10^{-6} n^2}{0.511 Z^2 (27.212)} \left(w_1^2 + w_2^2 - 2 w_1 w_2 \cos\theta\right). \tag{3}$$

In eq. (3), if energies w_1 and w_2 of the incident and scattered photon are expressed in eV, k comes out in atomic units. Obviously, θ represents the photon scattering angle. In this unit, the projection q of initial electron momentum on the scattering vector is given by

$$q = \frac{nw}{27.212\, kZ} - \frac{kZ}{2n} \tag{4}$$

with the energy transfer $w = w_1 - w_2$. The expression for the $1s$ profile is given by

$$J_{1s}^{EH} = \frac{256 k^3}{3Z}\left[1 - e^{-\frac{2\pi}{p}}\right]^{-1} \frac{1 + 3k^2 + p^2}{\left[(1 + k^2 - p^2)^2 + 4p^2\right]^3} \exp\left[\frac{-2}{p}\tan^{-1}\frac{2p}{1 + k^2 - p^2}\right] \tag{5}$$

where

$$p^2 = 2\left|\frac{n^2 w}{27.212\, Z^2} - \frac{}{2}\right. \tag{6}$$

The expressions for the $2s$ and $2p$ profile are also equally simple but somewhat lengthy. For a given incident photon energy w_1 and scattering angle θ the energy w_2 of the outgoing photon can be determined for various values q by using the result

$$w^2 = \frac{2w_1}{2\alpha + \beta^2 q^2 + \beta q(4\alpha + \beta^2 q^2)^{\frac{1}{2}}} \tag{7}$$

with

$$\alpha = 1 + \frac{2w_1 \sin^2 \frac{\theta}{2}}{511000} \tag{8}$$

and

$$\beta = \frac{2 \sin \frac{\theta}{2}}{137.036}. \tag{9}$$

The above analysis completes the formalism necessary for computing values of $J_{nl}^{EH}(q)$ as a function of q. For clarity of presentation, we have written eqs. (2), (4) and (6) in terms of atomic number Z. Since we are working within the framework of a screened hydrogenic model, the quantity Z should, in fact, be replaced by the effective nuclear charge (Z_{eff}) appropriate to the particular subshell under consideration. Also the (Z_{eff}) of the continuum electron (c) will enter into the expression for the exact Compton-profile. For the bound state electron (b), we shall use the values of Z_{eff} chosen in such a way that the impulse hydrogenic profiles for these states match the respective Hartee Fock profiles at the center, $q = 0$. The problem of obtaining Z_{eff}^{c} is a far more difficult problem. In their discussion of the photoeffect, Bethe and Salpeter [7] (while recognising that $Z_{eff}^{c} \to 0$ as $r \to \infty$) point out that since the greatest contribution to the matrix element occurs for distances of the order of the bound electron's Bohr radius, the most preferable choice is to set $Z_{eff}^{c} = Z_{eff}^{b}$

The impulse profile $J_{nl}^{I}(q)$ as a function of q is symmetric about $q = 0$ and has a maximum there. As opposed to this, the maximum of $J_{nl}^{EH}(q)$ computed from (2) occurs at q values not equal to zero. In other words, the maxima shift slightly (δq) either towards left ($-\delta q$) or towards right ($+\ \delta q$). The quantity δq is often termed as the Compton defect. We are interested in studying the K and L-shell Compton defects of MoK_α radiation ($w_1 = 17.374\ eV$) scattered through an angle $\theta = 155^\circ$. Using the chosen effective nuclear charges, we have computed the number for $J_{nl}^{EH}(q)$ as a function of q and noted down the values of δq where the exact profile exhibits a maximum. The result for δq and $J_{nl}^{EH}(q)$ for various Z are shown in Table 1.

The specific results presented include 1s, 2s and $2p^{(av)}$ profile values. The $2p$ impulse profile seems to average the $2p^{(\pm 1)}$ and $2p^{(0)}$ exact results. Since there are four electrons in the $2p^{(\pm 1)}$ state and two electrons in the $2p^{(0)}$ state, we have computed the $2p^{(av)}$ result by using the formula

$$J_{2p^{(av)}}^{EH}(q) = \frac{1}{3}\left[2J_{2p^{(\pm)}}^{EH}(q) + J_{2p^{(0)}}^{EH}(q)\right] \tag{10}$$

Table 1. Values of δq and $J_{nl}^{EH}(\delta q)$ in au.

sub-shell	1s		2s		2p	
Element	δq	$J_{1s}^{EH}(\delta q)$	δq	$J_{2s}^{EH}(\delta q)$	δq	$J_{2p(av)}^{EH}(\delta q)$
He	− 0.02	0.5330				
Li	0 06	0 3250	− 0 01	1 3852		
Be	− 0 11	0 2320	− 0 02	1.3352		
B	− 0 17	0 1794	− 0 03	0 9821		
C	− 0 23	0 1450	− 0 05	0 7935	0 21	0 4822
N	− 0.29	0 1203	− 0 07	0.6612	0.24	0.4252
O	− 0 31	0 1018	− 0 10	0 5632	0 27	0 3768
F	− 0.33	0 0868	− 0 13	0 4899	0.29	0 3367
Ne			− 0 16	0 4340	0 31	0 3030
Na			− 0 21	0 3689	0.35	0.2527
Mg			− 0 26	0 3232	0.37	0 2184
Al			− 0 31	0.2817	0 37	0 1928
Si			− 0 37	0 2521	0 38	0.1710
P			− 0 42	0 2290	0 39	0 1529
S			− 0 48	0.2081	0 43	0 1370
Cl			− 0 54	0 1872	0 51	0 1222
Ar			− 0 60	0 1732	0 67	0 1076

and have noted the corresponding position of the maxima accordingly. As expected, the values of δq for $1s$ and $2s$ subshell are negative while those for $2p^{(av)}$ are positive confirming the expectation of Mukhopadhyaya *et al* [4] and of Bell [8]. Both for s and p electrons $|\delta q|$ increases as Z increases. We have found that our numbers for δq are in exact agreement with those obtained by the approximation method of Holm and Ribberfors [9]. This implies that the so-called first correction to the impulse approximation is good enough at the MoK_α energy. The correction introduced by Holm and Ribberfors is essentially a high energy approximation of the exact profile. For example, if we assume that the energy and momentum transfer involved are large relative to the characteristic energy and momentum of the bound-state, then the wave vector $\boldsymbol{p}$ of the final state electron is a large quantity and we have the following results

$$\exp\left[-\frac{2}{p}\tan^{-1}\left(\frac{2p}{1+k^2-p^2}\right)\right]=1+\frac{2}{p}\tan^{-1}\nu \tag{11}$$

with

$$\nu = k - p$$

$$\left[(1+k^2-p^2)^2+4p^2\right]^3 = 64p^6(1+\nu^2)^3 \tag{12}$$

$$\left[1-e^{-\frac{2\pi}{p}}\right]^{-1} = \frac{p}{2\pi} \tag{13}$$

and

$$1+3k^2+p^2=4p^2\left(1+\frac{3v}{4p}\right). \tag{14}$$

In view of (11-14) the high energy result of $J_{1s}^{EH}(q)$ comes out in the form

$$J_{2s}^{EH}(q)=\frac{8}{3\pi Z(1+v^2)^3}\left[\frac{k}{p}\right]^3\left[1+\frac{2}{p}\tan^{-1}v+\frac{3v}{2p}\right]. \tag{15}$$

Within a normalisation factor, this high energy result has essentially been used by Holm and Ribberfors [9] for estimating the first order corrections to the impulse profile. However, at low energies an exact calculation like that of ours may turn out to be unavoidable. The values of $J_{nl}^{EH}(\delta q)$ for the $1s$ orbital are given for atoms, He ($Z=2$) to F ($Z=9$), because for $Z>9$ the conservation of energy leads to such a cut off on the negative wings of the Compton profiles, that does not permit one to investigate the maxima there. With Bloch and Mendelsohn [6] we have explicitly included this point in our calculation. The q cutoff has been determined by using the formula

$$q=\frac{X-\alpha}{\beta\sqrt{X}}, \tag{16}$$

where

$$X=\frac{w_1}{w_2} \tag{17}$$

The expressions for $J_{nl}^{EH}(q)$ given by Bell [8] are very simple and appear to be quite convenient to study profile asymmetries and Compton defects with particular emphasis on relative deviation (R) of the exact profile from the corresponding impulse result. We have verified that the mathematical expressions of Bell can be obtained from those in [6] quoted in this work by means of straightforward algebraic simplification.

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